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Spurious Oscillations in Computing Microstructures

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1. Introduction

The purpose of this paper is to discuss some numerical difficulties in a two-dimensional mathematical model for displacive phase transformations. For the physical and mathematical background see [1] [2] [4] [5] [6] [7] [9] [10] [8] [11] [12] . The usual approach to discretizing this model uses finite elements. Some previous work has computed certain microstructures by using a uniform square mesh discretization together with a form of derivative averaging. The overall scheme is equivalent to using bilinear elements with a one point quadrature approximation to discretize the energy functional E below. The resulting functional will be denoted by E_h. Although the square mesh respects a key symmetry property of the energy functional, when using this technique we have found a computational 'skewing' problem. This problem has a deleterious effect on the numerical solutions since it generates a grid scale spurious oscillation. In this paper, we will study this skewing phenomenon and attempt to show its effect on the computed microstructure.

Let $U : \Omega \to \mathbf{R}^2$ denote the deformation, where $\Omega = (0,1) \times (0,1)$. Then the energy functional has the form

$$E(U) = \int_\Omega W(\nabla U) dx.$$

An often used energy density is the Ericksen-James energy density:

$$W(F) = k_1(TrC - 2)^2 + k_2 c_{12}^2 + k_3\left((\frac{c_{11} - c_{22}}{2})^2 - \epsilon^2\right)^2,$$

where $C = F^t F$.

To avoid the small parameter ϵ, we use a new energy density in our computation:

$$W(F) = k_1(TrC - \alpha - \beta)^2 + k_2 c_{12}^2 + k_3(c_{11} - \alpha)^2(c_{22} - \alpha)^2.$$

This functional is frame indifferent and has the same right symmetry group (generated by $\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$) as the original functional. The two energy wells are generated by the action of SO_2 on

$$F_0 = \begin{pmatrix} \sqrt{\beta} & 0 \\ 0 & \sqrt{\alpha} \end{pmatrix}, \quad F_1 = \begin{pmatrix} \sqrt{\alpha} & 0 \\ 0 & \sqrt{\beta} \end{pmatrix}.$$

Continuity between two linear vector functions U_0 and U_1 requires the rank one connection

$$\nabla U_0 - \nabla U_1 = \mathbf{a} \otimes \mathbf{n},$$

where $\mathbf{n}$ is the normal of the interface. While F_0 and F_1 do not satisfy this equation, we can find a rotation R, such that

$$RF_1 - F_0 = \mathbf{a} \otimes \mathbf{n},$$

where

$$R = \begin{pmatrix} cos\theta & -sin\theta \\ sin\theta & cos\theta \end{pmatrix}, \quad \mathbf{n} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

$$sin\theta = -\frac{\alpha^2 - \beta^2}{\alpha^2 + \beta^2}, \quad cos\theta = \frac{2\alpha\beta}{\alpha^2 + \beta^2}.$$

Using the boundary condition $\frac{1}{2}(F_0 + RF_1)\mathbf{x}$, we would like to compute a continuous piecewise linear vector function U^h (depending on the mesh size h), which has the microstructure illustrated in Figure 1. But with the square mesh, the best numerical result we can expect is a staircase structure illustrated in Figure 2.

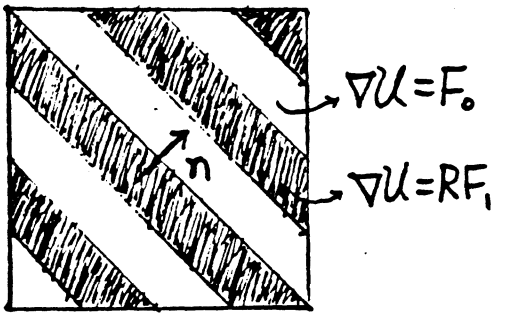


Figure 1.

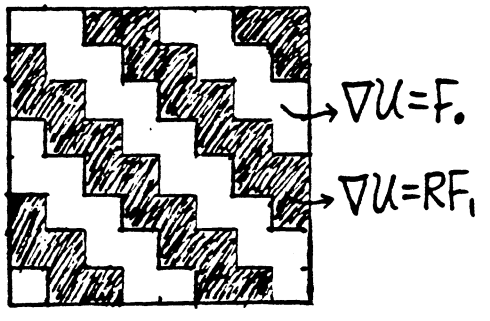
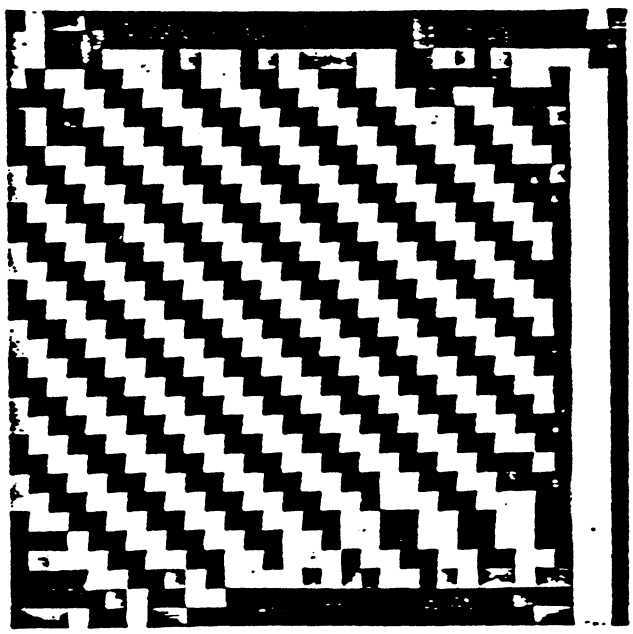


Figure 2.

Figure 3 plots a computed gradient distribution of U^h obtained by minimizing the energy $E_h(U^h)$. White colored squares denote well F_0 and black squares denote well RF_1. Other colors are not in wells (somewhere between F_0 and RF_1).



$\alpha = 5, \beta = 1, k_1 = 10, k_2 = 1, k_3 = 10, h = 1/32.$

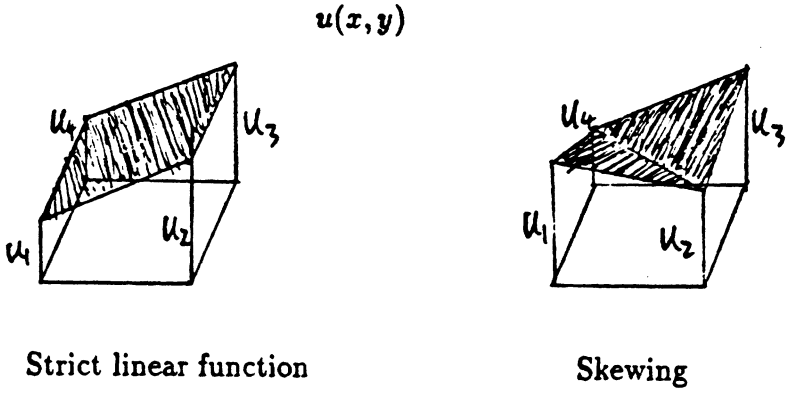
Figure 3.

2. SKEWING

Rank one connectivity requires that any two linear vector functions with gradients F_0 and RF_1 respectively, can only be patched along a straight line with the nomal $\mathbf{n}^t = (1,1)$. Therefore there is no piecewise linear vector function U such that ∇U equals F_0 and RF_1 within such staircase bands. In view of this, we need to look more closely at how the microstructure in Figure 3 is formed.

Let $U = \begin{pmatrix} u(x,y) \\ v(x,y) \end{pmatrix}$. We choose $u(x,y)$ and $v(x,y)$ to be piesewise linear functions. On each square element, u and v each have four (dependent) corner values. Let us consider u. Assume u equals u_1, u_2, u_3, u_4 on four corners over a square element (see Figure 4). Unless u is strictly linear, $\frac{u_2-u_1}{h} \neq \frac{u_3-u_4}{h}$. So naturally we use $u_x = \frac{1}{2}(\frac{u_2-u_1}{h} + \frac{u_3-u_4}{h})$ for ∇U, i.e. u_x equals to the average of lower side derivative and upper side derivative. Since the energy $E(U)$ only involves ∇U, we are able to form and minimize $E_h(U^h)$ by using this approximation for ∇U. In the minimization process, we adjust four values of u (same for

v) on each element to get average derivatives u_x and u_y which fall in one of two wells and provide small values for $E_h(U^h)$. This approach can overcome the rank one connectivity requirement by ignoring the linearity of u and v. The microstructure in the Figure 3 was obtained in this way. Figure 5 plots $u(x,y)$ over part of Ω. The skewing ('bending' along diagonals of squares) is obvious in this figure.



Strict linear function Skewing

Figure 4.

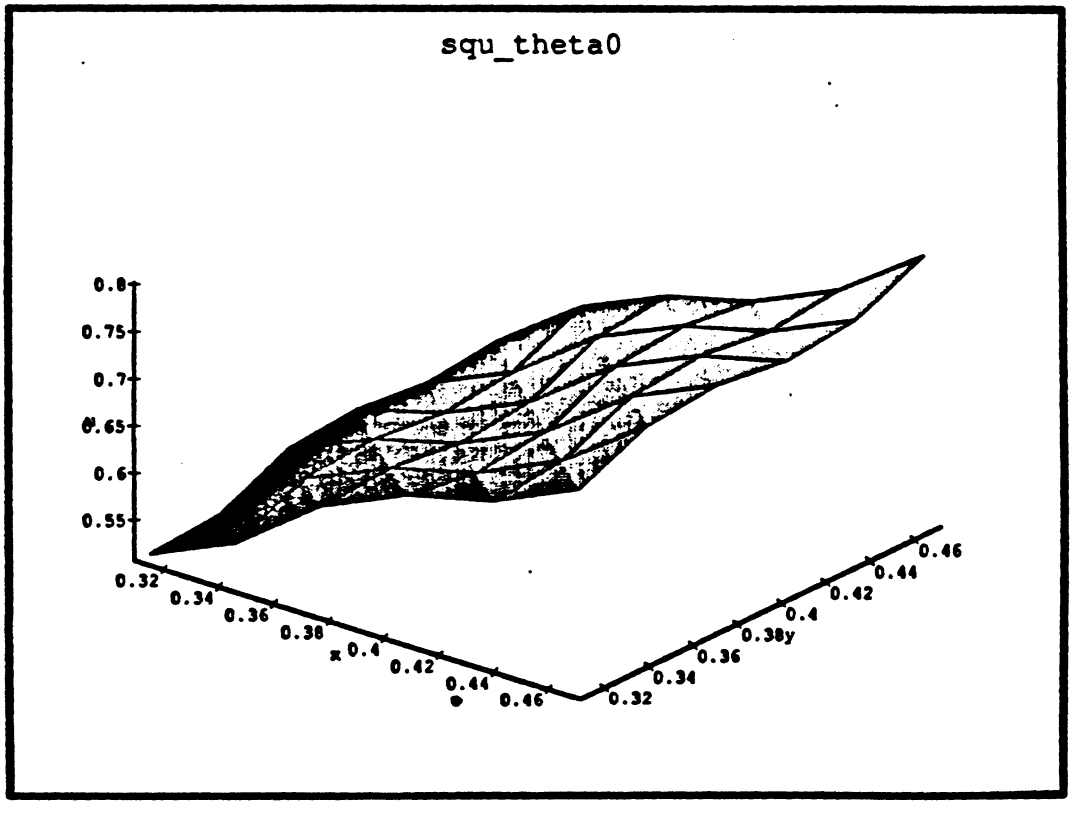


Figure 5.

If we rotate the domain by 45° to let the mesh orientation fit the twin plane normal, the effect of skewing can be more serious. Let $Q = \begin{pmatrix} \cos\frac{\pi}{4} & -\sin\frac{\pi}{4} \\ \sin\frac{\pi}{4} & \cos\frac{\pi}{4} \end{pmatrix}$. Now we expect to get a U^h which has roughly the following microstructure (ignoring boundary layers) :

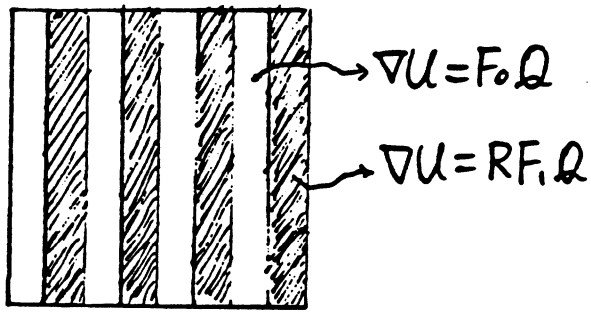


Figure 6.

Skewing does not greatly affect the value of $E_h(U^h)$. To illustrate this, consider Figure 7 and 8. In Figure 7 we plot $u(x,y)$ over part of Ω adjacent to the boundary $y = 0$. Figure 8 is the projection of ∇U^h onto the energy wells. In this figure, there should be a 'boundary layer' near $y = 0$, but it does not form. These figures suggest that the skewing allows ∇U^h to be in a well, even though U^h itself is not likely to be a good minimizer.

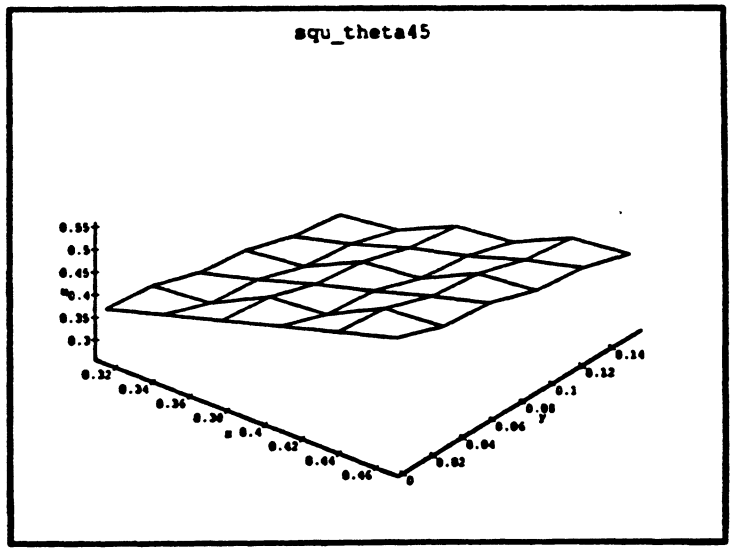
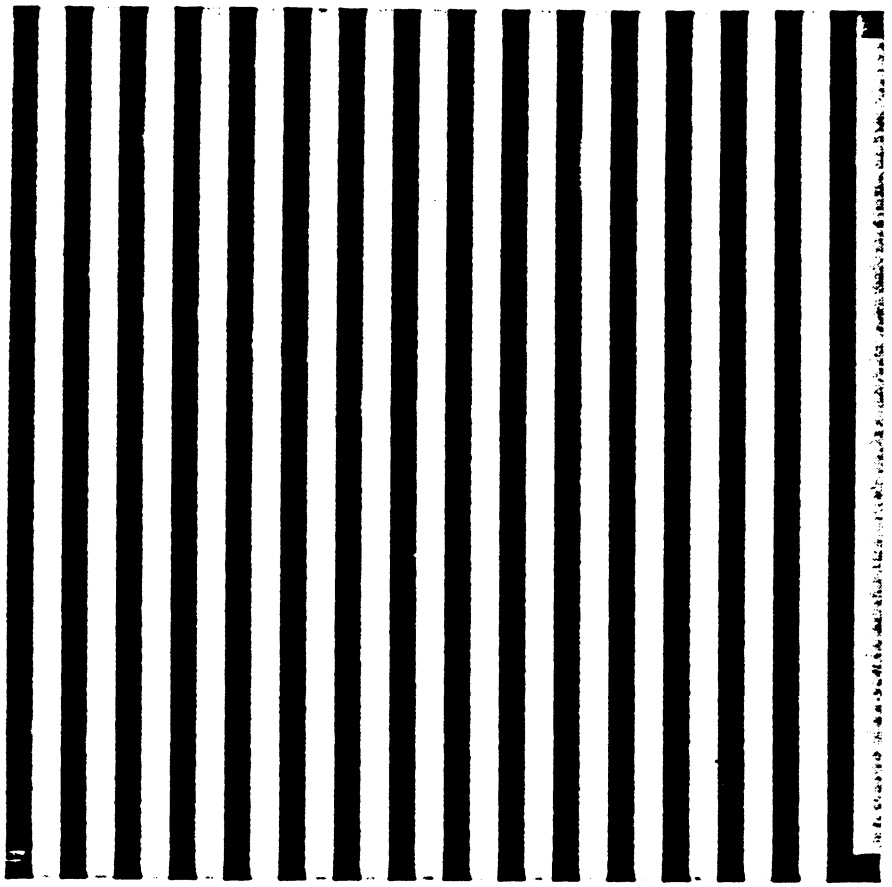


Figure 7.



$\alpha = 5, \beta = 1, k_1 = 10, k_2 = 1, k_3 = 10, h = 1/32.$

Figure 8.

There is a way to check this. Introduce a penalty term in the functional which penalizes skewing. It is as follows (restricted to one element) :

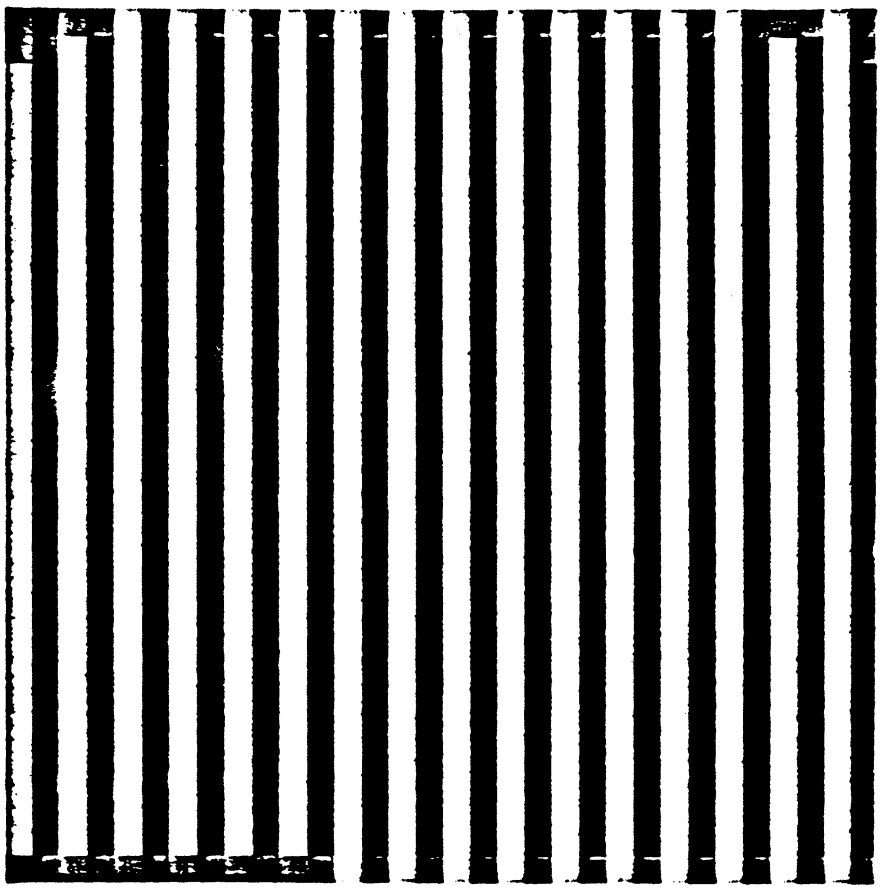
$$W[(u_2 - u_1) - (u_3 - u_4)]^2 + W[(v_2 - v_1) - (v_3 - v_4)]^2,$$

where W is a constant weight. Minimizing $E_h(U)$+*penalty term* produces a solution without noticeable skewing. Next we formed bilinear vector fields U with the computed values and computed the exact energy (using high order Gauss quadrature) of these fields. The results are as follows

	Standard Approach	Penalized Approach
Exact $E(U)$	140.64	18.33
Approx. $E_h(U^h)$	0.501	1.13

The exact energy of the skewed solution is relatively large, indicating that skewing exacts a severe energy penalty, even though the discretized functional suggests that the skewed solution is better. [1]

Figure 9 shows the microstructure of the penalized solution. The microstructure is similar to that of the skewed solution (Figure 8) except it has a 'boundary layer'. Comparing with Figure 7, Figure 10 plots the penalized $u(x,y)$ over the same region in Ω. It is indeed unskewed except near the boundary.



$\alpha = 5, \beta = 1, k_1 = 10, k_2 = 1, k_3 = 10, h = 1/32. \quad W = 10^4.$

Figure 9.

[1] The corresponding exact energy and approximate energy for the staircase microstructure in Figure 3 are 598.36 and 4.81.

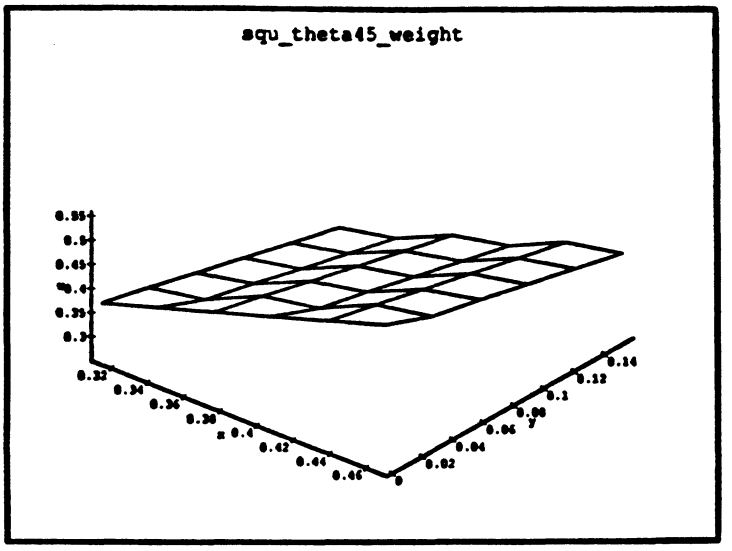


Figure 10.

We emphasize that we are not advocating the penalty technique as a general approach. It is merely a device to obtain an unskewed solution to compare with the skewed solution for the particular test problem considered here.

Skewing is not a novel phenomenon in numerical analysis. For example,[3] contains a detailed analysis of a closely similar effect for the stationary Stokes equations of fluid mechanics. It is shown in [3] that it is not sufficient to inhibit just the basic checkerboard mode. There are numerous other high frequency oscillations which contaminate the solution. In sufficiently simple cases these can be post processed to leave a more reliable solution. But this is not a very general approach.

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